Computer and Information Sciences
Modeling and Simulation

Data Discovery from Petascale Combustion Science Simulations

New computational capabilities aide in the development of efficient, clean burning engines and fuels.

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Combustion currently provides 85% of our nation's energy needs and will continue to be the predominant source of energy for the near term as the world transitions away from fossil fuels. Transportation is the second largest consumer of energy in the US and there are opportunities for improvements in efficiency of 25-50% through strategic technical investments in fuel and engine concepts and devices. High efficiency low-temperature engine concepts of the future operate in regimes where combustion is poorly understood, and experimentation provides only partial information. Thus, high performance computer simulation at the petascale (10^{15} operations/sec) provides the potential to revolutionize the way we optimize the design of future efficient, clean burning devices that make use of diverse future fuel sources and new combustion concepts.

Over the past several years, through sponsorship from the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Chemical Sciences, Geosciences, and Biosciences and the Office of Advanced Scientific Computing Research, scientists at Sandia's Combustion Research Facility (CRF) have performed and archived a library of direct numerical simulation (DNS) configurations and parametric studies addressing fundamental 'turbulence-chemistry' topics. These terascale (10^{12} operations/sec) studies, enabled by compute time granted under the Innovative and Novel Computational Impact on Theory and Experiment Program, have resulted in a profusion of high-dimensional, complex data. Figure 1 is a multi-variate volume visualization made possible through collaboration with the DOE SciDAC Ultrascale Visualization Institute that demonstrates a recent simulation of a lifted ethylene jet flame, consisting of 1.28 billion grid points and 22 chemical species that resulted in O(300) terabytes being written to disk [Reference 1]. Traditional analysis and visualization algorithms do not extend to inputs of this size, making it challenging to identify, classify, and track complex intermittent features in the resulting data.

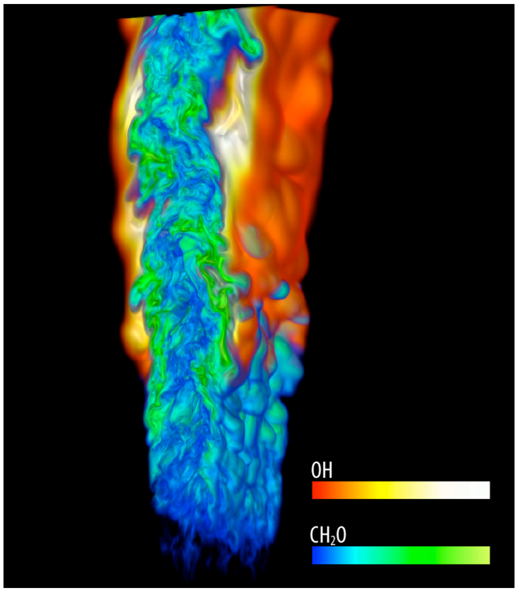

Figure 1: DNS of a lifted ethylene/air jet flame at Reynolds Number 10000. The hydroxyl radical (red/white) denotes the lifted flame whereas formaldehyde (blue/green) denotes ignition intermediates upstream of the lifted flame. Volume rendering courtesy of Hongfeng Yu of Sandia.

Towards this end, scientists at the CRF are developing a suite of tools that aide the exploration of DNS data. For example, COMPARED (Combined particle analysis, reduction, exploration, and display) [Reference 2] is a system for managing and performing categorization of large-scale data in a distributed environment that was used to encapsulate the Lagrangian view of autoignition shown in Figure 2. Scalar data is studied using tools from combinatorial topology such as the merge tree, which can be used to identify isovalues of interest on

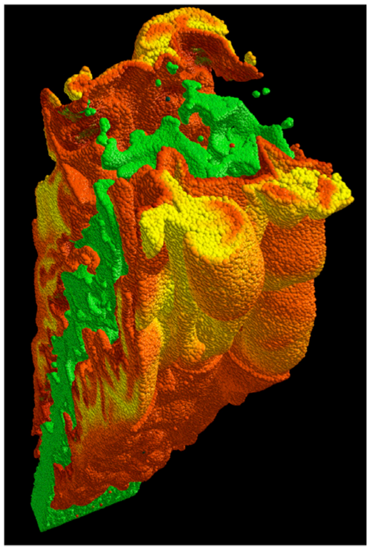

Figure 2: A Lagrangian view of autoignition. Particles in the raw fuel stream are colored by temperature from cold (green) to hot (red). The jet is issuing from the bottom left corner and flows towards the top of the figure.

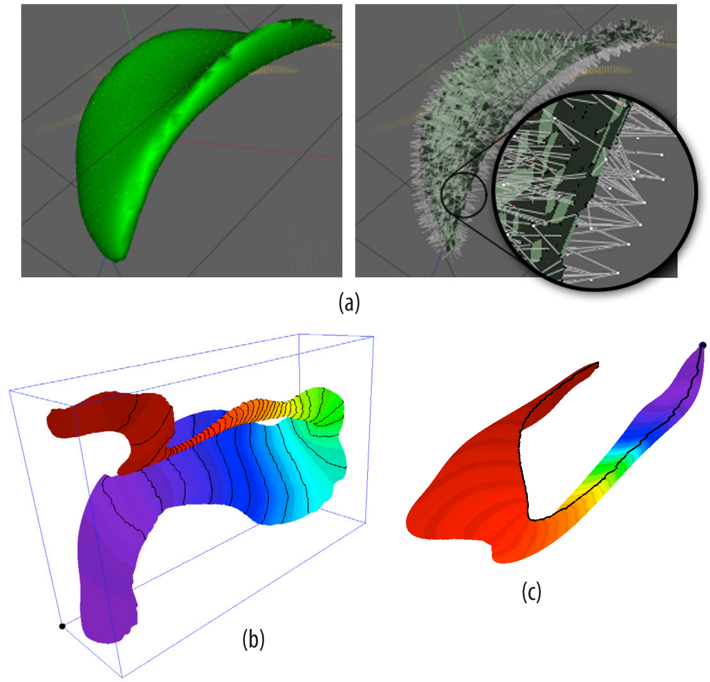

Figure 3: The morphology of the χ structures is studied using several metrics. In (a), the thickness distribution is computed as the distance from the medial axis. In (b) and (c), eigen analysis is performed to obtain circumference distributions and a length measure from the first non-trivial eigen vector of the graph Laplacian of the surface.

which to segment the data [Reference 3]. Figure 3 illustrates thin 'pancake-like' structures segmented from the scalar dissipation rate field χ that are subjected to compressive strain by the turbulence in the system. Scientists are interested in the morphology of the χ structures and current research efforts include the development of appropriate shape analysis metrics. Topological analysis is also used to study the relationship between scalar fields. Figure 4 corresponds to a DNS of a lifted autoigniting turbulent jet flame in a hot air coflow, used to investigate the physics of lifted flame stabilization in the presence of ignition. Topological analysis confirms that the χ field and the HO_2 ignition kernels, a marker of ignition, overlap with low probability in regions upstream of the lifted flame base.

Efforts are underway to deploy these tools, together with others currently under development, in a unified framework so that metrics of interest can be studied and explored by scientists, providing fundamental insights necessary to address our nation's current energy needs.

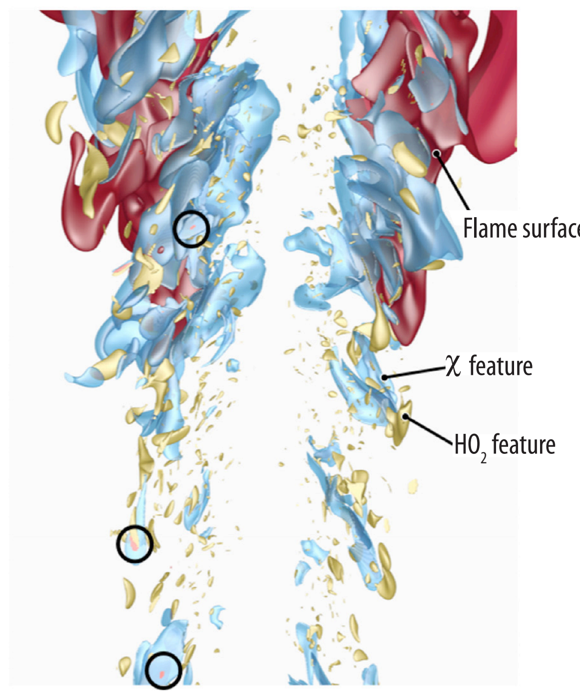

Figure 4: The topological analysis confirms that the χ features (blue) and HO_2 ignition kernels (yellow) overlap with very low probability in the region upstream of the lifted flame base (red). Those regions that overlap greater than a particular threshold have been circled.

References

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3. Topological Feature Extraction for Exploration of Terascale Combustion Data, A. Mascarenhas, R. W. Grout, P.-T. Bremer, E. R. Hawkes, V. Pascucci, J. H. Chen, in Topoinvis '09: Topological Methods in Data Analysis and Visualization, Snowbird, Utah, February 23-24, 2009.

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